

Free-energy transition in a gas of non-interacting nonlinear wave-particles

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We investigate the dynamics of a gas of non-interacting particle-like soliton waves, demonstrating that phase transitions originate from their collective behavior. This is predicted by solving exactly the nonlinear equations and by employing methods of the statistical mechanics of chaos. In particular, we show that a suitable free energy undergoes a metamorphosis as the input excitation is increased, thereby developing a first order phase transition whose measurable manifestation is the formation of shock waves. This demonstrates that even the simplest phase-space dynamics, involving independent (uncoupled) degrees of freedom, can sustain critical phenomena.

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The methods of statistical mechanics have permeated physics as a whole including modern areas of deterministic chaos [1], complexity [2], and nonlinear waves [3, 4, 5]. Among its basic notions, it is well known that the thermodynamics associated to a gas of non-interacting particles is trivial, being characterized by a constant free-energy with respect to control parameters. Conversely, in order to have cooperative phenomena, such as phase-transitions or more complex processes, the intervention of some sort of interaction potential must be called for.

Within the context of nonlinear wave propagation, a challenge to the generality of this picture could come from *solitons*, i.e. exact solutions of integrable nonlinear partial differential equations (PDE), which display well-known particle-like behavior. Stemming from the numerical experiments of Fermi-Pasta-Ulam (FPU) on the equipartition of energy in nonlinear chains [6], solitons have found applications in areas as different as Bose-Einstein condensation (BEC) [7], nonlinear optics [8, 9], fluid-dynamics [10], solid state physics [11], general relativity [12] and many others. While relying on large (non-perturbative) nonlinear effects, solitons conserve their number and spectral parameters (eigenvalues) evolving without any practical interaction, albeit some displacements in their collisions. The isospectrality allows for reducing the infinite-dimensional phase space associated to the global wave-function to a simple one where N independent degrees of freedom corresponding to N soliton particles are effective. On this basis one can argue whether the statistical description of an ensemble of *non-interacting* solitons is actually as trivial (i.e., with a constant free energy and no critical phenomena) as inferred from the statistical mechanics of free particles, or else exhibits cooperative phenomena as the number of particles (degrees of freedom) grows. In this Letter, we address this issue by investigating the statistical mechanics of a gas of soliton particles. By exploiting ideas from the thermostatics of chaos [1], we demonstrate that a suit-

ably defined free-energy undergoes a metamorphosis as the number of solitons grows, changing from a constant to a function that supports a first-order phase transition. Correspondingly, the overall wave-function develops a steep front (shock), which results from the scaling properties of the soliton velocity distribution, in turn determined by the input excitation. Hence the shock formation can be interpreted as a cooperative process of several solitons. Therefore even the simplest phase-space dynamics, where particle-like waves evolve independently from the others, could result into phase-transitions.

We make reference to a universal integrable model, namely the defocusing nonlinear Schrödinger equation:

$$i\frac{\partial\psi}{\partial z} - \frac{\partial^2\psi}{\partial x^2} + 2(|\psi|^2 - \rho^2)\psi = 0, \quad (1)$$

and by means of the inverse scattering transform (IST) [13], we calculate the field evolution after the so-called *dark* initial condition $\psi(x, 0) = -\rho \tanh x$, with ρ integer. The latter is experimentally accessible and particularly important in BEC and nonlinear optics [7, 8, 9], where the occurrence of dispersive shock waves has been recently observed and discussed [14, 15, 16, 17, 18, 19], though in regimes not involving dark disturbances and the soliton-driven wave-breaking discussed here. The constraint ρ =integer, corresponding to a *reflectionless* potential, allows us to investigate a novel scenario where the dispersive shock dynamics is determined solely by solitons that are embedded in the input, with radiation waves playing absolutely no role. Unlike previous approaches to shock waves (hydrodynamic limit, Whitham averaging) involving different degrees of approximation [19, 20, 21, 22, 23], we derive exact solutions of Eq. (1), which enable us to contrast the smooth dynamics determined by a small number N of solitons with the strongly nonlinear case ($\rho, N \gg 1$). In the latter regime, this approach allows us to introduce a free energy that reflects the spectral distribution of solitons in the (invariant) eigenvalue space, using a non-canonical measure [1].

In this respect, our approach shows no similarities with the Gibbsian statistical mechanics of soliton-bearing systems where nonlinear excitations are thermally controlled [3, 4], or with the kinetic theory of random distributions of colliding solitons [5]. Our formulation is general and applies to every integrable system, such as integrable versions of FPU.

Spectral transform. — The solution of Eq. (1) is derived by means of IST in two steps: (i) by calculating the spectral transform of the system; (ii) by solving the inverse scattering problem. It is worth to remark that the solution of Eq. (1) with initial value $\psi_0 = \psi(x, 0)$ represents a far more general problem than the calculation of the generic N -soliton solution of Eq. (1). The former, in fact, calls for the evaluation of the spectral transform $\mathcal{S}\{\psi_0\}$ of ψ_0 and the solution of the inverse problem for $\mathcal{S}\{\psi_0\}$, while the latter needs just the calculation of the inverse problem for an unknown ψ whose spectrum contains only solitons. In order to highlight the main physical results, we defer unessential mathematical details to an extended publication, while referring to Ref. [13] for the IST method. The spectral transform $\mathcal{S}\{\psi_0\}$ is defined as:

$$\mathcal{S}\{\psi_0\} = \{-\infty < \lambda < \infty, \frac{b(\lambda)}{a(\lambda)}; \lambda_n, c_n, n = 1, \dots, N\}, \quad (2)$$

with the reflection coefficient $b/a = R$, λ_n corresponding to simple zeros of a (for $\text{Im}(\lambda) \geq 0$) and $c_n = b(\lambda_n)/\dot{a}(\lambda_n)$, being λ a spectral parameter and $a(\lambda)$, $b(\lambda)$ transition coefficients relating the Jost solutions of the direct scattering problem [13]. We calculate a and b corresponding to ψ_0 , obtaining:

$$a = i \frac{k \cdot \Gamma(\frac{k}{2i})^2}{\lambda \cdot \Gamma(\frac{k}{2i} + \rho) \Gamma(\frac{k}{2i} - \rho)}, \quad b = \frac{k \cdot |\Gamma(i\frac{k}{2})|^2}{2\Gamma(1 - \rho) \Gamma(\rho)}. \quad (3)$$

When ρ is integer, $R = 0$ and ψ_0 is a reflectionless potential containing $N_\rho \equiv N(\rho) = 2\rho - 1$ solitons. The spectral transform $\mathcal{S}\{\psi_0\}$ then reads:

$$\mathcal{S}\{\psi_0\} = \{R(\lambda) = 0; \lambda_{\pm n} = \pm 2\sqrt{\rho^2 - (\rho - n)^2}, c_{\pm n} = (-1)^{n+1} \frac{\prod_j (s_{\pm n} - s_j^*)}{\prod_{j \neq \pm n} (s_{\pm n} - s_j)}, n = 0, \dots, M\}, \quad (4)$$

with $s_n = \lambda_n + 2i(\rho - n)$, $j \in [-M, M]$ and $M \equiv \rho - 1$.

Inverse scattering problem. — The z -evolution of the wave function ψ is found from the solution of the inverse problem [13] and, for the spectral transform represented by Eq. (4), reads:

$$\psi(x, z) = \rho \left[1 + \frac{|B|}{|A|} \right], \quad B = \begin{bmatrix} A & e \\ d & 0 \end{bmatrix}, \quad (5)$$

where $d_l = i\sqrt{c_l/s_l}e^{\nu_l(x - \lambda_l z)/2}$, $e_j = i2\rho d_j/s_j$, $j, l \in [-M, M]$, $\nu_j \equiv 2(\rho - j)$ and A is the matrix

$$A_{jl} = \delta_{jl} + i \frac{2\rho \sqrt{c_j \bar{c}_l} e^{[x(\nu_l + \nu_j) - z(\nu_l \lambda_l + \nu_j \lambda_j)]/2}}{\sqrt{s_j \bar{s}_l} (s_j - s_l^*)}. \quad (6)$$

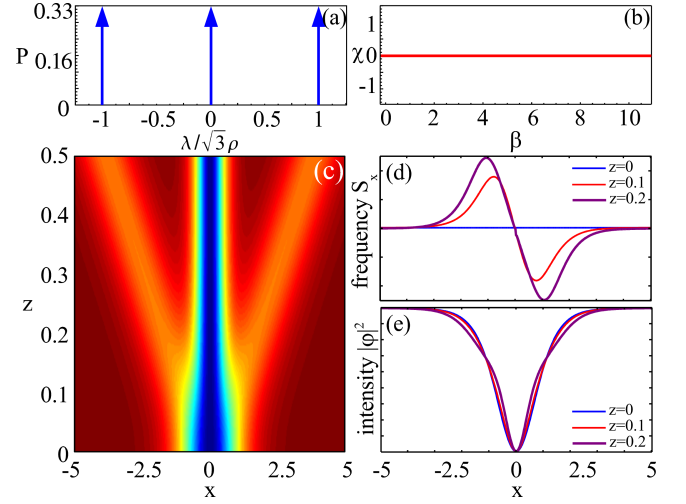


FIG. 1: (Color online) 3-dark soliton solution corresponding to $\psi_0 = 2 \tanh x$: (a) Eigenvalue measure P (p_j/ϵ for $\epsilon \rightarrow 0$); (b) numerically calculated free energy \mathcal{X} vs. β ; (c) Pseudo-color level plot of intensity $|\psi|^2$; (d)-(e) Profiles of frequency S_x and intensity $|\psi|^2$ at different z .

Equations (4) and (5) describe the soliton evolution corresponding to the input ψ_0 . Note that λ_n represent the invariant velocity of the n -th soliton.

Soliton-gas thermodynamics. — To derive a soliton-gas thermodynamics, we begin by decomposing the spectral transform $\mathcal{S}\{\psi_0\}$ as the sum of spectral transforms of individual solitons (normal modes):

$$\mathcal{S}\{\psi_0\} = \sum_{j=-M}^M \{R(\lambda) = 0; \lambda_j, c_j\} = \sum_{j=-M}^M \mathcal{S}\{\phi_j\}, \quad (7)$$

with λ_j and c_j given by (4). A remarkable property of integrable PDE is that each conserved quantity of the system, such as the energy or the momentum, follows the decomposition (7) and can be expressed as the sum of conserved quantities of individual solitons. By exploiting this property, we evaluate the Hamiltonian H :

$$H = \int_{-\infty}^{\infty} dx \left[\left| \frac{\partial \psi}{\partial x} \right|^2 + (|\psi|^2 - \rho^2)^2 \right] = \sum_{j=-M}^M \frac{\nu_j^3}{3}, \quad (8)$$

whose explicit summation yields $H = \frac{4}{3}\rho^2(\rho^2 + 1)$, i.e. the Hamiltonian of $\psi = \psi_0 = -\rho \tanh x$. Equation (8) states that the system can be regarded as a gas of non-interacting particles possessing a purely kinetic Hamiltonian of the form $H = \sum_j m v_j^2/2$, with mass $m = 2/3$ and equivalent velocities $v_j = \nu_j^{3/2}$. The latter governs the observable dynamics in the “dual space” of the wave-function ψ , through Eqs. (5-6).

The thermodynamics of such soliton gas can be studied by means of *escort distributions* [1]. Given an arbitrary measure, whose representative microstates have probability p_i , escort distributions are constructed from the Lie

transformation group $P_k = f(p_k, \beta) = p_k^\beta / \sum_j p_j^\beta$. The connection with statistical mechanics is derived by defining the partition function $Z(\beta) = \sum_j p_j^\beta = \exp(-\Psi)$, correspondingly $P_i = \exp(\Psi - \beta \mathcal{E}_i)$, $\mathcal{E}_i = -\ln p_i$ being the energy of the i -th microstate, and $\beta = 1/T > 0$ the inverse “temperature”. The Helmholtz free energy is given by $F(\beta) = \Psi/\beta$. We define the phase-space as the range $[-1, 1]$ of $\lambda/2\rho$. As a principal measure of the soliton gas, we consider its eigenvalue distribution $\lambda_i/2\rho$, which is at the basis of the evolution in the dual wavefunction space through Eq. (5). We then partition the phase-space in $N_\epsilon = 2/\epsilon$ boxes of size ϵ , and define p_i as the normalized ($\sum_j p_j = 1$) probability of finding an eigenvalue in the interval $[-1 + (i-1)\epsilon, -1 + i\epsilon]$ with $i = 1, 2, \dots, N_\epsilon$. Following the thermostatics of multifractals [1], we study the thermodynamic limit of F , defined by

$$\beta \mathcal{F} = \mathcal{X} = \lim_{V \rightarrow \infty} \frac{\Psi}{V} \quad (9)$$

being $V = -\ln \epsilon$ the “volume”. Correspondingly, when $\epsilon \rightarrow 0$, the partition function scales as $Z \sim \epsilon^\chi$.

Thermodynamic limit for small particle densities. — We begin by calculating \mathcal{X} when the amplitude ρ is small enough so that the N_ρ eigenvalues λ_j are well separated in the spectrum. This situation corresponds to a low density soliton gas. In this case, the probability p_j of finding an eigenvalue in the j -th box of width ϵ is either 0 or $1/N_\rho$. Therefore, in the limit $\epsilon \rightarrow 0$, the non-vanishing p_j scales as ϵ^0 , since each eigenvalue occupies a single point in the gap $|\lambda/2\rho| \leq 1$. The partition function then reads

$$Z = \sum_j^{N_\epsilon} p_j^\beta = N_\rho \left(\frac{1}{N_\rho} \right)^\beta = N_\rho^{1-\beta} \sim \sum_j^{N_\rho} \epsilon^0 \sim \epsilon^{\mathcal{X}(\beta)}. \quad (10)$$

This yields a very simple thermodynamics, where both \mathcal{X} and \mathcal{F} are zero, with the distribution function P of the eigenvalues, determined as the limit of p_j/ϵ for $\epsilon \rightarrow 0$, being a set of Dirac delta (Fig. 1a,b). The resulting wave evolution is smooth, without the formation of any singular behavior. We specifically address the case of $\rho = 2$, where the results of the IST analysis are manageable to be reported in simple closed form. Equation (5) yields the particular 3-dark soliton solution relative to eigenvalues $0, \pm 2\sqrt{3}$ as a function of $X \equiv 2x, \zeta \equiv 4\sqrt{3}z \in [0, \infty)$:

$$\psi = \frac{4(\cosh \zeta + \cosh X + i\sqrt{3} \sinh \zeta) \sinh X}{-3 - 4 \cosh \zeta \cosh X - \cosh 2X}. \quad (11)$$

Figures 1c-e display the level plot evolution of the intensity or density (in BEC) $|\psi|^2$, and snapshots of $|\psi|^2$ and $S_x = \partial S / \partial x = \text{Im}\{\psi_x / \psi\}$. The generation of three dark solitons by ψ_0 does not lead to the formation of steep fronts during propagation: each soliton slowly splits up from the others throughout the process, from the initial overlap state (i.e., at $z = 0$ the particles occupy the

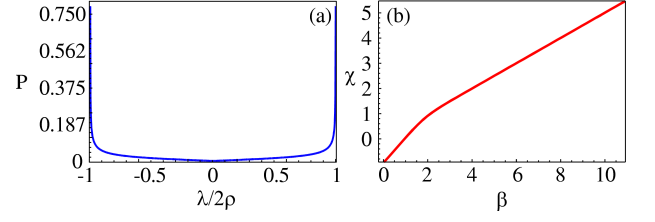


FIG. 2: (Color online). (a) Eigenvalue measure P (for $\epsilon \rightarrow 0$) versus $\lambda/2\rho$ for a dense gas; (b) Free energy \mathcal{X} versus inverse temperature β .

same position $x = 0$) to the asymptotic stage where they are well separated. As stated above, this relies on the absence of phase transitions in soliton gas (Fig. 1a-b), owing to a constant free energy landscape $\mathcal{F} = 0$. In summary, cooperative phenomena and shocks are prohibited at small input amplitudes ρ , or equivalently, for low density soliton gases where $\mathcal{F} = 0$.

Thermodynamics for dense soliton gases. — When the number of eigenvalues λ grows large for $\rho \gg 1$, the soliton ensemble turns into a dense gas and the eigenvalue distribution $\lambda/2\rho = \pm\sqrt{1 - (1 - n/\rho)^2}$ becomes a continuous function of the variable n/ρ . The density of the positive eigenvalues $\mathcal{D}(\lambda/2\rho)$ is readily seen to be $\mathcal{D}(y) = y/2\sqrt{1 - y^2}$ and, correspondingly, it is found that

$$p_j = \sqrt{1 - (j-1)^2\epsilon^2} - \sqrt{1 - j^2\epsilon^2}. \quad (12)$$

For $\epsilon \rightarrow 0$, we identify three different scaling regimes in Eq. (12): (i) $p_j \propto \epsilon^2$ for $\lambda \cong 0$; (ii) $p_j \propto \epsilon$ for $\lambda \cong \rho$; (iii) $p_j \propto \sqrt{\epsilon}$ for $\lambda \cong 2\rho$, with the partition function Z scaling as

$$Z = \sum_j p_j^\beta \sim (N_\epsilon - 3)\epsilon^\beta + 2\epsilon^{\beta/2} + \epsilon^{2\beta} \quad (13)$$

with two boxes near $\lambda = \pm 2\rho$ scaling like $\epsilon^{\beta/2}$, one near $\lambda \cong 0$ scaling like $\epsilon^{2\beta}$ and the remaining $N_\epsilon - 3$ scaling like ϵ^β . In the limit $\epsilon \rightarrow 0$, we can actually neglect the contribution of $\epsilon^{2\beta}$ (as the probability $p_j \cong 0$ for $\lambda \cong 0$). The partition function then reads $Z \sim \epsilon^{\beta-1} + \epsilon^{\beta/2} \sim \epsilon^\chi$. This implies $\mathcal{X} = \min[\beta - 1, \beta/2]$ and leads to:

$$\mathcal{X} = \begin{cases} \beta - 1, & \beta \leq \beta_c \\ \frac{\beta}{2}, & \beta > \beta_c \end{cases} \quad (14)$$

being $\beta_c = 2$ the critical point such that $\beta_c - 1 = \beta_c/2$. Equation (14) states that the system undergoes a first-order phase transition as the inverse temperature β is varied, since the free energy $\beta \mathcal{F} = \mathcal{X}$ is continuous but not differentiable at β_c . As seen in Fig. 2b, \mathcal{X} and P calculated numerically after the expression of the eigenvalue λ_n support this picture. Such a phase transition is the main mechanism leading to shock formation in the dual space of wave dynamics. In fact, owing to the different

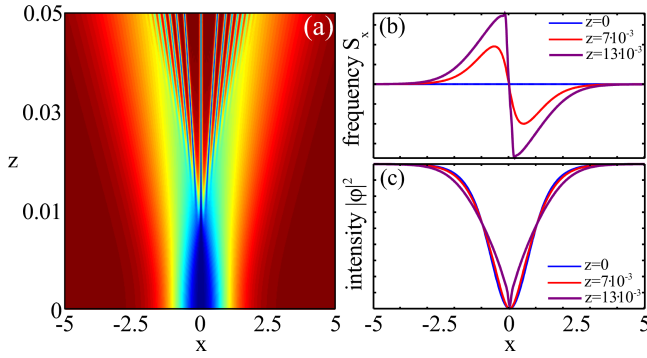


FIG. 3: (Color online). (a) Level plot of intensity $|\psi|^2$, and (b) snapshots of frequency S_x and (c) intensity $|\psi|^2$, for input $\psi_0 = 30 \tanh x$.

scaling of p_j , wave-particles with close but opposite soliton velocities λ_j tend to be accumulated at gap edges; starting from the initial overlap state, such process generates a nearly discontinuous variation in the overall frequency S_x . To illustrate this dynamics, we calculate the evolution of a dense soliton gas corresponding to $\rho = 30$ (Fig. 3). A dramatic variation of S_x is observed for $z = z^* \approx 0.013$ (Fig. 3b), with a shock (steep front) in $x = 0$ eventually originating from a compressional-like wave ($S_x > 0$ for $x < 0$ and viceversa), beyond which fast oscillations in x appear. Each oscillation is indeed associated with a wave particle (dark soliton), with solitons splitting up in pairs with opposite velocities around a central black ($\lambda = 0$) soliton (Fig. 3a). Correspondingly, the intensity $|\psi|^2$ becomes singular in z^* (Fig. 3c). The dynamics of ψ in the dense case ($\rho = 30$) is dramatically different if compared to the 3-soliton case (see Figs. 1c-d and 3b-c): the absence of cooperative phenomena when the number of soliton is small, in fact, does not lead to any singular behavior (shock wave) in the field propagation along z . We emphasize that, despite solitons tend to split up from the beginning ($z = 0$) due to their different velocities, their collective behavior results, owing to the compressional wave feature, into a dramatic focusing of the dark notch intensity, which turns out to be an easily measurable signature of the critical behavior. Remarkably this occurs while: (i) no radiation is involved; (ii) the phase space supporting the gas dynamics is composed by non-interacting particles. In summary, a dense gas of noninteracting soliton wave-particles turns out to support critical phenomena. The latter originates from a singularity of the free-energy, which undergoes a metamorphosis as the number of soliton grows and develops a first-order phase transition. As shown, the relevant order parameter for the soliton gas transition is the shape of the function $\beta\mathcal{F}$, which changes with the input excitation.

In conclusion, we have illustrated a scenario where the

formation of a dispersive shock wave involves only solitons. In spite of the fact that solitons behave as non-interacting particles with well-defined parameters, they do not follow the canonical behavior of systems with non-interacting degrees of freedom. Rather their cooperation leads to measurable critical phenomena characterized by a free energy that develops a singularity when the number of solitons grows sufficiently large. This finding can stimulate both novel experiments and new ideas in the field of statistical mechanics of nonlinear waves.

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